Influence of the Third Dimension of Quasi-2D Cuprate Superconductors on Angle-Resolved Photoemission Spectra

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We discuss how the effects of dispersion of electronic states with \$k z\$, which have largely been neglected in discussing the cuprates, play out in the analysis and interpretation of the angle-resolved photoemission (ARPES) spectra from quasi-2D materials. Illustrative results on Bi\$ 2\$Sr\$ 2\$CaCu\$ 2\$O\$ {8}\$ (Bi2212) and La\$ {2-x}\$Sr\$ x\$CuO\$ 4\$ (LSCO) are presented. \$k z\$dispersion induces an irreducible width to ARPES spectral peaks which does not have its origin in a scattering mechanism. It is also manifest in ARPES photointensities for emission from the Fermi energy, where the Fermi surface maps so obtained display \$k \parallel\$-dependent widths, which can be quite large especially in the antinodal region. The first principles photointensities computed in LSCO within the local-density approximation (LDA) based band theory framework are found to reproduce many salient features of the experimental ARPES spectra, even in the underdoped regime, suggesting that a remnant of the quasi-particle continues to persist even in the presence of strong electron correlations, albeit with a reduced spectral weight. In the lightly doped insulating LSCO, we show via tight binding model computations that effects of \$k z\$-dispersion can give insight into the characteristic broadenings observed in the ARPES features associated with the lower Hubbard band and the mid-gap states.